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Ab initio treatment of electron correlations in polymers: lithium hydride chain and beryllium hydride polymer

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Correlated *ab initio* electronic structure calculations are reported for the polymers lithium hydride chain $[LiH]_\infty$ and beryllium hydride $[Be_2H_4]_\infty$. First, employing a Wannier-function-based approach, the systems are studied at the Hartree-Fock level, by considering chains, simulating the infinite polymers. Subsequently, for the model system $[LiH]_\infty$, the correlation effects are computed by considering virtual excitations from the occupied Hartree-Fock Wannier functions of the infinite chain into the complementary space of localized unoccupied orbitals, employing a full-configuration-interaction scheme. For $[Be_2H_4]_\infty$, however, the electron correlation contributions to its ground state energy are calculated by considering finite clusters of increasing size modelling the system. Methods such as Møller–Plesset second–order perturbation theory and coupled–cluster singles, doubles and triples level of theory were employed. Equilibrium geometry, cohesive energy and polymerization energy are presented for both polymers, and the rapid convergence of electron correlation effects, when based upon a localized orbital scheme, is demonstrated.